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Local Structure about I Atoms in Iodinated YBCO Single Crystals Determined by I- L_3 edge EXAFS Analysis.

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Beamline(s): X19A

Introduction: The recovery of superconductivity in underdoped (insulating) of $YBa_2Cu_3O_{6+y}$ ($y \leq 0.6$) by halogernation has not been well understood. A location of halogen atoms is also a controversial issue. Recently we have reported on polarized multiple-edge EXAFS studies of normal and brominated YBCO single crystals [1] having T_c~63 and 89K, respectively. The brominated sample becomes strongly heterogeneous on the atomic length scales. Br does not enter substitutionally or interstitially into the perfect YBCO structure, but occupies Cu(1) site in nano-fragments of YBCO lattice forming Br-O(4)-Ba-Cu2(1)-Cu(1)-… nano-clusters. This work is undertaken to explore the local structure about the iodine in iodinated YBCO (y~0.4) single crystal, showing T_c~ 70K.

Methods and Materials: Diffraction patterns of the iodinated crystal revealed no evidence of the secondary phases. I L_3- edge polarized EXAFS spectra were collected at X19A in FY, using a 13-element Ge detectors with energy resolution of ~260 eV. All spectra were recorded at room temperature.

Results: The major peak in the FT of the EXAFS spectrum can be satisfactory fitted assuming contributions from one Ba atom at ~3.50±0.03 Å, two Cu atoms at ~3.70±0.03 Å and one Cu atom at ~4.16±0.05 Å. Note that the extracted distances similar to those expected for Cu(1)-Ba, Cu(1)-Cu(2), and Cu(2)-Cu(1) distances in YBCO lattice. However, the coordination numbers are strongly reduced, indicating that iodine does not enter the perfect YBCO lattice. The shape of clusters about the iodine is determined by analyzing all possible scenarios. Firstly, the lattice of iodinated sample is fragmented. Secondly, it has to be randomly oriented with respect of the "crystal". EXAFS fit over a range of 0.8-4.5 Å (in the *R*-space) may be further improved by adding two contributions: One is from the oxygen neighbors at ~1.81 Å (I-O(4) coordination number is somewhat smaller than expected value of ~1). Another one is due to one Cu atom at ~2.45 Å. The latter contribution appears to come from nano copper iodine (since no traces of CuI is found by long-range order sensitive x-ray diffraction measurements). No appreciable number of I-O(1) pairs (*R*~1.94 Å) is detected, implying that O(1) could being liberated and, therefore, made available for re-oxygenation of the underdoped unreacted regions. The local structure about the I is consistent with the cluster expansions of I-Ba-Cu2(1)-Cu(1)-… and I-Cu-…
It worth noticing that the extracted interatomic distances of I-X [X=Ba,Cu(2), and Cu(1)] rule out any interstitial location of iodine in the YBCO lattice.

Conclusions: We found that iodination gives rise to the changes in the local structure of YBCO that are results in very similar to those in brominated YBCO [1]. Iodine does not enter intertitially or substitutionally into the perfect lattice. It forms nano-clusters of I-Ba-Cu2(1)-Cu(1)-…, liberating oxygen, and apparently re-oxygenating the underdoped regions. Cu *K*-edge EXAFS measurements have to be done to support the re-oxygenation of the "host" lattice accommodating the nano-clusters.

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References: [1] L. M. Dieng, A. Yu. Ignatov, T. A. Tyson, M. Croft, F. Dogan, C. -Y. Kim, J. C. Woicik and J. Grow, "Observation of Changes in the Atomic and Electronic Structure of Single-Crystal $YBa_2Cu_3O_{6.6}$ Accompanying Bromination", Phys. Rev. B **66**, (2002), *014501-014513*.